



Simulation of supercritical water–hydrocarbon mixing in a cylindrical tee at intermediate Reynolds number: Impact of temperature difference between streams



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ABSTRACT

The objective of this work is to study the impact of the temperature difference between the streams on the flow dynamics and mixing of supercritical water (SCW) and a model hydrocarbon (n-decane), under fully miscible conditions, in a small-scale cylindrical tee mixer (pipe ID = 2.4 mm), at an intermediate inlet *Reynolds number* of 500 using 3-D CFD simulations. When the water and n-decane streams enter the mixer at inlet temperatures of 800 K and 700 K respectively ($\Delta T = 100$ K), the flow remains laminar and the variations of density and viscosity with temperature do not have a significant impact on the flow and mixing dynamics. However, when the water inlet temperature is 1000 K ($\Delta T = 300$ K), the water–HC shear layer becomes unstable close to $x = 5D$ downstream of the mixing joint followed by shear-layer rollup and transition to turbulence. This leads to significant enhancement in the mixing rate. However, in a simulation of SCW n-decane mixing with the same inlet conditions but with the physical properties held fixed at the inlet values (no variation with temperature), the shear layer remains stable and steady state is reached. It was found that, the large variation of temperature of 300 K within the mixing layer leads to an increase in the local fluid density and a decrease in the local fluid viscosity within the mixing layer attributed mainly to the cooling of water and the heating of n-decane respectively. These physical property variations result in an increase in the local Reynolds number within the shear layer rendering it unstable to perturbations in the flow. Thus, the variations in mixture density and viscosity with temperature under near-critical conditions were found to have a significant impact on the flow and mixing dynamics in the tee mixer.

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1. Introduction

The current study builds on the foundations laid in a previous work [1], in which, we formulated and applied a numerical model for the simulation of supercritical water and hydrocarbon mixing in a 3-D cylindrical tee mixer with a consistent treatment of near-critical thermodynamic and transport property variations. In that study, for a temperature difference of 100 K between the water and hydrocarbon streams, the resultant physical property variations did not have a significant impact on the flow field. In the present work, we focus on the effect of the temperature difference (ΔT) between the hydrocarbon and water streams on the flow field and mixing dynamics in a cylindrical tee mixer under fully miscible conditions and at intermediate Reynolds numbers.

The effect of temperature difference between the two streams on the mixing process arises due to the substantial variation of fluid physical properties with temperature under near-critical conditions. The physical property gradients can influence the local flow stability as also promote the development of vortical structures leading to faster mixing. Previous studies in literature have investigated the effect of physical property gradients due to differences in properties of the two pure mixing streams on flow stability and mixing structures. Miller et al. [2] performed direct numerical simulations (DNS) of a supercritical heptane–nitrogen temporal mixing layer (both two and three dimensional) and studied the effect of density stratification across the shear layer on the transition to turbulence. Okong'o et al. [3] performed a similar DNS of a supercritical liquid oxygen/hydrogen three dimensional mixing layer and observed a similar effect of the density stratification causing a suppression of the transition to turbulence. They investigated this effect by looking at the vorticity budget. Zong et al. [4] have performed the LES of a two-dimensional cryogenic

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supercritical nitrogen jet at high Re and studied the spatial and temporal evolution of the jet for different ambient pressures which lead to varying amounts of density stratification. Their findings seem consistent with previous results of Miller et al. [2] and Okong'o et al. [3] regarding the effect of density stratification leading to the suppression of shear layer transition to turbulence. Soteriou et al. [5] numerically investigated the effects of the free-stream density ratio on the evolution of incompressible, high Reynolds and Froude number, confined mixing layer and established that a non-unity density ratio alters the flow characteristics by influencing the entrainment patterns by means of baroclinic generation of vorticity. Li et al. [6] performed a direct simulation of nitrogen jet injection in the close vicinity of the critical point at a Reynolds number of 1750. They found that the shear layer was disturbed by volume dilatation and the baroclinic torque generated made the layer more unstable. These effects also stimulate the vortex rolling up and pairing processes.

The effect of temperature of the water medium surrounding a hydrocarbon droplet on the mixing of the two has been studied in the works of Dabiri et al. [7] and Wu et al. [8]. In the 1-D spherically symmetric simulations of water–toluene and water–decane mixing, the water temperature being below the upper critical solution temperature (UCST) of the binary system retards the mixing rate due to the prolonged persistence of the phase interface. Wu et al. [8] extended this numerical framework to ternary water–HC–HC systems of water–toluene–decane and water–toluene–tetralin. They demonstrated an interesting fractionation effect (selective buildup of one of the hydrocarbons in the water phase) when the water temperature is between the UCSTs of the two different water–HC binary systems (UCST of water–toluene system is 308 °C while UCST of water–decane system is 359 °C). These studies have provided useful insight and know-how on the modeling methods for near-critical water–hydrocarbon flows for the current study. The formulation and methodology developed for simulating mixing of near-critical fluids in complicated 3-D geometries reported in [1] are employed in this study. The focus is on the mixing of water and a model hydrocarbon (n-decane) under fully miscible conditions (above the UCST) in a cylindrical tee mixer geometry at intermediate Reynolds numbers with emphasis on the impact of near-critical property variations due to temperature gradients on the flow field stability and mixing dynamics.

This paper starts with a discussion of the governing equations pertinent to this study in Section 2. Then, the modeling of near-critical thermodynamic behavior and transport property variations is outlined in Section 3. This is followed by an explanation of the mixer geometry and boundary conditions in Section 4. The results of the numerical simulations are then presented and discussed in detail in Section 6. Finally, the conclusions of this study are summarized in Section 7.

2. Governing equations

The conservation equations used to simulate the mixing of supercritical water and hydrocarbon (here, n-decane) are given below in Eqs. (1)–(5), in the most general form in order to accommodate variable density, compressibility and variable transport property effects. Since the equations are solved numerically using a finite-volume (FV) formulation, they are expressed in the strong conservative form. The assumptions employed in the formulation of these equations are explained in detail in a previous work [1].

Continuity Equation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 \quad (1)$$

Momentum Equation (Navier–Stokes):

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_j u_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i \quad (2)$$

where the stress tensor (τ_{ij}) is given by:

$$\tau_{ij} = 2\mu \left(S_{ij} - \frac{1}{3} S_{ii} \delta_{ij} \right) = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} \frac{\partial u_i}{\partial x_i} \quad (3)$$

where μ is the viscosity of the mixture (calculated using the methodology outlined in Section 3)

Species Transport Equation:

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_j Y_k}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D_k \frac{\partial Y_k}{\partial x_j} \right) \quad (4)$$

where, the subscript k denotes species k , Y_k is the mass fraction of species k in the mixture and D_k is the mass diffusivity of species k in the bulk mixture.

Enthalpy Transport Equation:

$$\begin{aligned} \frac{\partial \rho h}{\partial t} + \frac{\partial \rho u_j h}{\partial x_j} &= \frac{DP}{Dt} + \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) \\ &+ \sum_k \frac{\partial}{\partial x_j} \left(h_k \rho D_k \frac{\partial Y_k}{\partial x_j} \right) + \tau_{ij} \frac{\partial u_i}{\partial x_j} \end{aligned} \quad (5)$$

3. Thermodynamics and transport properties

The Peng–Robinson equation of state in conjunction with the standard van der Waals mixing rules was used to model the thermodynamics of the binary water–HC system and is given below:

$$P = \frac{R_u T}{V - b_m} - \frac{a_m}{V^2 + 2b_m V - b_m^2} \quad (6)$$

$$a_m = \sum_i \sum_j x_i x_j (1 - k_{ij}) \sqrt{a_i a_j} \quad (7)$$

$$b_m = \sum_i x_i b_i \quad (8)$$

where a_i and b_i for each species in the mixture are calculated using its critical temperature (T_{ci}), critical pressure (P_{ci}) and acentric factor (ω_i):

$$\begin{aligned} a_i &= 0.457236 \frac{R_u^2 T_{ci}^2}{P_{ci}} \left[1 + \left(0.3746 + 1.5423 \omega_i \right. \right. \\ &\quad \left. \left. - 0.2699 \omega_i^2 \right) \left(1 - \sqrt{\frac{T}{T_{ci}}} \right) \right]^2 \end{aligned} \quad (9)$$

$$b_i = 0.0777961 \frac{R_u T_{ci}}{P_{ci}} \quad (10)$$

In Eq. (7), k_{ij} is a binary interaction parameter for the species pair i and j . The binary interaction parameter for the species pair was calculated using a predictive Peng–Robinson (PPR78) approach with a group contribution method (GCM) [9]. The details of the thermodynamic calculations are presented in a previous work [1]. The viscosity and thermal conductivity of the pure components are calculated using the generalized correlations of Chung et al. [10]. The value of the mixture viscosity and thermal conductivity is taken to be a mass fraction-weighted average of the individual component properties as also done by Narayanan et al. [11] in their study. The mass diffusivity of the components in the mixture is calculated using the Tracer Liu–Silva–Macedo (TLSM) model [12–14].

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